Search Page 13

WEST Search History

DATE: Friday, August 09, 2002

Set Name side by side	Query	Hit Count	Set Name result set
	DB=USPT,PGPB,JPAB,EPAB,DWPI; PLUR=YES; OP=ADJ		
L3	L1 same polymorphism	9	L3
L2	L1 same polymorphism	9	L2
L1	(polypeptide or protein) same (predict$ near3 structure)	1992	L1

END OF SEARCH HISTORY

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Search Results - Record(s) 1 through 9 of 9 returned.

☐ 1. Document ID: US 20020106742 A1

L3: Entry 1 of 9 File: PGPB Aug 8, 2002

PGPUB-DOCUMENT-NUMBER: 20020106742
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20020106742 A1

TITLE: Nucleic acids encoding active and inactive CCR5 chemokine receptors

PUBLICATION-DATE: August 8, 2002

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY	RULE-47
Samson, Michel	Gentilly		FR	
Parmentier, Marc	Linkebeek		BE	
Vassart, Gilbert	Brussels		BE	
Libert, Frederick	Braine-L'Alleud		BE	

US-CL-CURRENT: 435/69.51; 435/320.1, 435/325, 435/5, 514/44, 530/350, 536/23.5

ABSTRACT:

A peptide has an amino acid sequence having more than 80% homology with the amino acid sequence listed as SEQ ID NO:4. A nucleic acid molecule has more than 80% homology with one of the nucleic acid sequences listed as SEQ ID NO:1, SEQ ID NO:2 and SEQ ID NO:3. Ligands, anti-ligands, cells vectors relating to the peptide and/or nucleic acid molecule are also used.

KWIK: Invalid display element.

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments | Claims | KWIC | Draw. Desc | Image

☐ 2. Document ID: US 20020094536 A1

L3: Entry 2 of 9 File: PGPB Jul 18, 2002

PGPUB-DOCUMENT-NUMBER: 20020094536
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20020094536 A1

TITLE: Methods for making polynucleotide libraries, polynucleotide arrays, and cell libraries for high-throughput genomics analysis

PUBLICATION-DATE: July 18, 2002

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY	RULE-47
Lofquist, Alan	Seattle	WA	US	
Finney, Robert E.	Seattle	WA	US	
Leung, David	Seattle	WA	US	

US-CL-CURRENT: 435/6; 435/287.2, 435/320.1

ABSTRACT:

A method for high-throughput, genomics analysis, to identify the therapeutic or diagnostic utility of genes, entails the use of a construct to disrupt a gene or alleles of a gene in cells of interest. Arrays of such cells can be used to monitor such disrupted cells phenotypically in the context, for example, of testing drug candidates. Polynucleotides that comprise part of the disrupted genes can be recovered from such "knockout" cells, by virtue of an origin of replication or a host cell selection marker sequence that is part of the construct. The recovered polynucleotides can be used to identify the disrupted genes or to make homologous recombination vectors, which in turn can be employed to make multi-allele knockout cells.

KWIK: Invalid display element.

☐ 3. Document ID: US 6331388 B1

L3: Entry 3 of 9 File: USPT

US-PAT-NO: 6331388
DOCUMENT-IDENTIFIER: US 6331388 B1

TITLE: Immune response enhancer

DATE-ISSUED: December 18, 2001

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Malkovsky; Miroslav	Madison	WI		
Wells; Andrew D.	Mt. Laurel	NJ		

US-CL-CURRENT: 435/5; 424/278.1, 435/375, 435/69.1, 435/7.21, 435/7.22, 435/7.23, 435/7.24, 435/7.31, 435/7.32, 514/44

ABSTRACT:

The present invention provides methods for specifically increasing expression of MHC class I molecules in cells, and in particular, in poorly immunogenic tumor cells as well as in pathogen-infected cells. Also provided by the present invention are methods for increasing presentation of endogenous antigens onto the cell surface by MHC class I molecules, as well as methods of increasing the immunity of an animal against an antigen. The methods presented herein are useful in enhancing immune recognition of any cell infected with any pathogen, for in vitro and in vivo screening of candidate immunogene therapeutic approaches, and for enhancing the generation of antibodies to an otherwise poorly immunogenic antigen or cell. The present invention further provides methods for reducing or increasing the radiation sensitivity of a cell.

14 Claims, 92 Drawing figures

Exemplary Claim Number: 1
Number of Drawing Sheets: 61
KWIK: Invalid display element.

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments KWMC | Draw. Desc | Image

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☐ 4. Document ID: US 6191268 B1

L3: Entry 4 of 9 File: USPT

US-PAT-NO: 6191268
DOCUMENT-IDENTIFIER: US 6191268 B1

TITLE: Compositions and methods relating to DNA mismatch repair genes

DATE-ISSUED: February 20, 2001

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Liskay; Robert M.	Lake Oswego	OR		
Bronner; C. Eric	Portland	OR		
Baker; Sean M.	Portland	OR		
Bollag; Roni J.	Martinez	GA		
Kolodner; Richard D.	Jamaica Plain	MA		

US-CL-CURRENT: 536/23.5; 536/24.3, 536/24.31, 536/24.33

ABSTRACT:

Genomic sequences of human mismatch repair genes are described, as are methods of detecting mutations and/or polymorphisms in those genes. Also described are methods of diagnosing cancer susceptibility in a subject, and methods of identifying and classifying mismatch-repair-defective tumors. In particular, sequences and methods relating to human mutL homologs, hMLH1 and hPMS1 genes are provided.

80 Claims, 16 Drawing figures
Exemplary Claim Number: 4
Number of Drawing Sheets: 25
KWIK: Invalid display element.

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments KWMC | Draw. Desc | Image

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☐ 5. Document ID: US 6165713 A

L3: Entry 5 of 9 File: USPT

US-PAT-NO: 6165713
DOCUMENT-IDENTIFIER: US 6165713 A

TITLE: Composition and methods relating to DNA mismatch repair genes

DATE-ISSUED: December 26, 2000

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Liskay; Robert M.	Lake Oswego	OR		
Bronner; C. Eric	Portland	OR		
Baker; Sean M.	Portland	OR		
Bollag; Roni J.	Martinez	GA		
Kolodner; Richard D.	Jamaica Plain	MA		

US-CL-CURRENT: 435/6; 435/7.1, 435/91.1, 435/91.2, 536/24.33

ABSTRACT:

Genomic sequences of human mismatch repair genes are described, as are methods of detecting mutations and/or polymorphisms in those genes. Also described are methods of diagnosing cancer susceptibility in a subject, and methods of identifying and classifying mismatch-repair-defective tumors. In particular, sequences and methods relating to human mutL homologs, hMLH1 and hPMS1 genes are provided.

55 Claims, 12 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 22
KWIK: Invalid display element.

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments

KWIC | Drawi Desc | Image

☐ 6. Document ID: US 5922855 A

L3: Entry 6 of 9 File: USPT

US-PAT-NO: 5922855
DOCUMENT-IDENTIFIER: US 5922855 A

TITLE: Mammalian DNA mismatch repair genes MLH1 and PMS1

DATE-ISSUED: July 13, 1999

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Liskay; Robert M.	Lake Oswego	OR		
Bronner; C. Eric	Portland	OR		
Baker; Sean M.	Portland	OR		
Bollag; Roni J.	Martinez	GA		
Kolodner; Richard D.	Jamaica Plain	MA		

US-CL-CURRENT: 536/23.5; 536/24.3, 536/24.31, 536/24.33

ABSTRACT:

We have discovered two human genes, hMLH1 and hPMS1, each of which apparently encodes for a protein involved in DNA mismatch repair. The hMLH1 gene encodes for a protein which is homologous to the bacterial DNA mismatch repair protein MutL, and is located on human chromosome 3p21.3-23. We believe that mutations in the hMLH1 gene cause hereditary non-polyposis colon cancer (HNPCC) in some individuals based upon the similarity of the hMLH1 gene product to the yeast DNA mismatch repair

protein MLH1, the coincident location of the hMLH1 gene and the HNPCC locus on chromosome 3, and hMLH1 missense mutations in affected individuals from a chromosome 3-linked HNPCC family. The human hPMS1 gene is homologous to the yeast DNA mismatch repair gene PMS1, and is located on human chromosome 7q. We believe that the hPMS1 gene is a strong candidate for HNPCC testing because the yeast proteins MLH1 and PMS1 have been shown to be involved in the same DNA repair pathway and because hMLH1 and hMSH2 have both been implicated in HNPCC families. The most immediate use for hMLH1 and hPMS1 will be in screening tests on individuals who are members of families which exhibit high frequencies of early onset cancer. We have also isolated and sequenced mouse MLH1 and PMS1 genes. We have produced chimeric mice with a mutant form of the PMS1 gene that will enable us to derive mice that are heterozygous or homozygous for mutation in mPMS1. These mice will be useful for cancer research. We have also produced and isolated antibodies directed to hPMS1 which are useful in assays to detect the presence of protein in tumor samples.

3 Claims, 16 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 17
KWIK: Invalid display element.

☐ 7. Document ID: US 5807732 A

L3: Entry 7 of 9 File: USPT

US-PAT-NO: 5807732
DOCUMENT-IDENTIFIER: US 5807732 A

TITLE: GDP-L-fucose: .beta.-D-galactoside 2-.alpha.-L-fucosyltransferases, DNA sequences encoding the same, method for producing the same and a method of genotyping a person

DATE-ISSUED: September 15, 1998

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Lowe; John B.	Ann Arbor	MI	48105	
Lennon; Gregory	Castro Valley	CA	94552	
Rouquier; Sylvie	34000 Montpellier			FR
Giorgi; Dominique	34000 Montpellier			FR
Kelly; Robert J.	Trenton	MI	48183	

US-CL-CURRENT: 435/358; 435/193, 435/252.2, 435/252.3, 435/320.1, 435/325, 435/365, 435/69.1, 536/23.2

ABSTRACT:

The gene encoding GDP-L-fucose: .beta.-D-Galactoside 2-.alpha.-L-fucosyltransferase has been cloned, and a mutation in this gene has been found to be responsible for an individual being a non-secretor.

12 Claims, 30 Drawing figures
Exemplary Claim Number: 9
Number of Drawing Sheets: 23
KWIK: Invalid display element.

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments KWIC | Draw. Desc | Image

☐ 8. Document ID: US 5703048 A

L3: Entry 8 of 9 File: USPT

US-PAT-NO: 5703048
DOCUMENT-IDENTIFIER: US 5703048 A

TITLE: Protection against liver damage by HGF

DATE-ISSUED: December 30, 1997

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Roos; Filip	Brisbane	CA		
Schwall; Ralph	Pacifica	CA		

US-CL-CURRENT: 514/12; 435/360, 514/2, 514/838, 514/893, 514/894, 530/350, 530/399

ABSTRACT:

The present invention provides methods for preventing occurrence or progression of liver damage using hepatocyte growth factor. In the methods, a preventatively effective amount of the hepatocyte growth factor is administered to the patient. The hepatocyte growth factor can be administered, for instance, prior to administering a hepatotoxic therapy to the patient. The hepatocyte growth factor can further be administered with activin or transforming growth factor-beta to prevent liver damage. Compositions comprising hepatocyte growth factor and activin antagonist or transforming growth factor-beta antagonist are also provided by the invention.

15 Claims, 9 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 5
KWIK: Invalid display element.

Full | Title | Citation | Front | Review | Classification | Date | Reference | Sequences | Attachments KWIC | Draw. Desc | Image

☐ 9. Document ID: US 5654404 A

L3: Entry 9 of 9 File: USPT

US-PAT-NO: 5654404
DOCUMENT-IDENTIFIER: US 5654404 A

TITLE: Protection against liver damage by HGF

DATE-ISSUED: August 5, 1997

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Roos; Filip	Brisbane	CA		
Schwall; Ralph	Pacifica	CA		

US-CL-CURRENT: 530/387.3; 424/134.1, 424/136.1, 424/178.1, 530/350

ABSTRACT:

The present invention provides methods for preventing occurrence or progression of liver damage using hepatocyte growth factor. In the methods, a preventatively effective amount of the hepatocyte growth factor is administered to the patient. The hepatocyte growth factor can be administered, for instance, prior to administering a hepatotoxic therapy to the patient. The hepatocyte growth factor can further be administered with activin or transforming growth factor-beta to prevent liver damage. Compositions comprising hepatocyte growth factor and activin antagonist or transforming growth factor-beta antagonist are also provided by the invention.

18 Claims, 9 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 5
KWIK: Invalid display element.

Term	Documents
POLYMORPHISM.DWPI,EPAB,JPAB,USPT,PGPB.	8755
POLYMORPHISMS.DWPI,EPAB,JPAB,USPT,PGPB.	6771
(1 SAME POLYMORPHISM).USPT,PGPB,JPAB,EPAB,DWPI.	9
(L1 SAME POLYMORPHISM).USPT,PGPB,JPAB,EPAB,DWPI.	9

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 NEWS  3  Apr 09   BEILSTEIN: Reload and Implementation of a New Subject Area
 NEWS  4  Apr 09   ZDB will be removed from STN
 NEWS  5  Apr 19   US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
 NEWS  6  Apr 22   Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
 NEWS  7  Apr 22   BIOSIS Gene Names now available in TOXCENTER
 NEWS  8  Apr 22   Federal Research in Progress (FEDRIP) now available
 NEWS  9  Jun 03   New e-mail delivery for search results now available
 NEWS 10  Jun 10   MEDLINE Reload
 NEWS 11  Jun 10   PCTFULL has been reloaded
 NEWS 12  Jul 02   FOREGE no longer contains STANDARDS file segment
 NEWS 13  Jul 22   USAN to be reloaded July 28, 2002;
                   saved answer sets no longer valid
 NEWS 14  Jul 29   Enhanced polymer searching in REGISTRY
 NEWS 15  Jul 30   NETFIRST to be removed from STN
 NEWS 16  Aug 08   CANCERLIT reload
 NEWS 17  Aug 08   PHARMAMarketLetter(PHARMAML) - new on STN
 NEWS 18  Aug 08   NTIS has been reloaded and enhanced
 NEWS 19  Aug 09   JAPIO to be reloaded August 18, 2002

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               CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),
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FILE 'BIOSIS' ENTERED AT 09:32:00 ON 09 AUG 2002
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=> s (predict? (3a) structure) and (protein or polypeptide)
L1 8344 (PREDICT? (3A) STRUCTURE) AND (PROTEIN OR POLYPEPTIDE)

=> s l1 and review/dt
L2 290 L1 AND REVIEW/DT

=> s l2 and fold?
L3 96 L2 AND FOLD?

=> duplicate remove l3
PROCESSING COMPLETED FOR L3
L4 96 DUPLICATE REMOVE L3 (0 DUPLICATES REMOVED)

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L4 ANSWER 1 OF 96 MEDLINE
AN 2002087866 MEDLINE
DN 21674677 PubMed ID: 11814876
TI Molecular modelling in structural biology.
AU Forster Mark J
CS Informatics Laboratory, National Institute for Biological Standards and Control, Blanche Lane, South Mimms, Hertfordshire, UK..
mfoster@nibsc.ac.uk
SO MICRON, (2002) 33 (4) 365-84. Ref: 154
Journal code: 9312850. ISSN: 0968-4328.
CY England: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, ACADEMIC)
LA English
FS Priority Journals
EM 200205
ED Entered STN: 20020130
Last Updated on STN: 20020509
Entered Medline: 20020508
AB Molecular modelling is a powerful methodology for analysing the three dimensional structure of biological macromolecules. There are many ways in which molecular modelling methods have been used to address problems in structural biology. It is not widely appreciated that modelling methods are often an integral component of structure determination by NMR spectroscopy and X-ray crystallography. In this review we consider some of the numerous ways in which modelling can be used to interpret and rationalise experimental data and in constructing hypotheses that can be tested by experiment. Genome sequencing projects are producing a vast wealth of data describing the **protein** coding regions of the genome under study. However, only a minority of the **protein** sequences thus identified will have a clear sequence homology to a known **protein**. In such cases valuable three-dimensional models of the **protein** coding sequence can be constructed by homology modelling methods. Threading methods, which used specialised schemes to relate **protein** sequences to a library of known structures, have been shown to be able to identify the likely **protein fold** even in cases where there is no clear sequence homology. The number of **protein** sequences that cannot be assigned to a structural class by homology or threading methods, simply because they belong to a previously unidentified **protein folding** class, will decrease in the future as collaborative efforts in systematic structure determination begin to develop. For this reason, modelling methods are likely to become increasingly useful in the near future. The role of the blind prediction contests, such as the Critical Assessment of techniques for **protein Structure Prediction** (CASP), will be briefly discussed. Methods for modelling **protein**-ligand and

protein-protein complexes are also described and examples of their applications given.

L4 ANSWER 2 OF 96 MEDLINE
AN 2002178153 MEDLINE
DN 21909381 PubMed ID: 11911887
TI Functional plasticity of CH domains.
AU Gimona Mario; Djinovic-Carugo Kristina; Kranewitter Wolfgang J; Winder Steven J
CS Department of Cell Biology, Institute of Molecular Biology, Austrian Academy of Sciences, Salzburg, Austria.. mgimona@server1.imolbio.oeaw.ac.at
SO FEBS LETTERS, (2002 Feb 20) 513 (1) 98-106. Ref: 55
Journal code: 0155157. ISSN: 0014-5793.
CY Netherlands
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200205
ED Entered STN: 20020326
Last Updated on STN: 20020508
Entered Medline: 20020507
AB With the refinement of algorithms for the identification of distinct motifs from sequence databases, especially those using secondary **structure predictions**, new **protein** modules have been determined in recent years. Calponin homology (CH) domains were identified in a variety of **proteins** ranging from actin cross-linking to signaling and have been proposed to function either as autonomous actin binding motifs or serve a regulatory function. Despite the overall structural conservation of the unique CH domain **fold**, the individual modules display a quite striking functional variability. Analysis of the actopaxin/parvin **protein** family suggests the existence of novel (type 4 and type 5) CH domain families which require special attention, as they appear to be a good example for how CH domains may function as scaffolds for other functional motifs of different properties.

L4 ANSWER 3 OF 96 MEDLINE
AN 2002101763 MEDLINE
DN 21674960 PubMed ID: 11814598
TI Structural proteomics: developments in **structure**-to-function **predictions**.
AU Norin Martin; Sundstrom Michael
CS Biovitrum, Department of Structural Chemistry., Stockholm, Sweden.
SO TRENDS IN BIOTECHNOLOGY, (2002 Feb) 20 (2) 79-84. Ref: 50
Journal code: 8310903. ISSN: 0167-7799.
CY England: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200204
ED Entered STN: 20020209
Last Updated on STN: 20020412
Entered Medline: 20020410
AB The major challenge for post-genomic research is to functionally assign and validate a large number of novel target genes and their corresponding **proteins**. Functional genomics approaches have, therefore, gained considerable attention in the quest to convert this massive data set into useful information. One of the crucial components for the functional understanding of unassigned **proteins** is the analysis of their experimental or modeled 3D structures. Structural proteomics initiatives

are generating **protein** structures at an unprecedented rate but our current knowledge of 3D-structural space is still limited. Estimates on the completeness of the 3D-structural coverage of **proteins** vary but it is generally accepted that only a minority of the structural proteome has a template structure from which reliable conclusions can be drawn. Thus, structural proteomics has set out to build a map of **protein** structures that will represent all **protein** **folds** included in the 'global proteome'.

L4 ANSWER 4 OF 96 MEDLINE
AN 2002074954 MEDLINE
DN 21661098 PubMed ID: 11802435
TI GTOP: database for **protein** 3D **structure** **prediction**.
AU Kawabata T; Nishikawa Ktakawaba@lab.nig.ac.jp
SO TANPAKUSHITSU KAKUSAN KOSO. PROTEIN, NUCLEIC ACID, ENZYME, (2001 Dec) 46 (16 Suppl) 2592-7. Ref: 12
Journal code: 0413762. ISSN: 0039-9450.
CY Japan
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA Japanese
FS Priority Journals
EM 200202
ED Entered STN: 20020125
Last Updated on STN: 20020227
Entered Medline: 20020226

L4 ANSWER 5 OF 96 MEDLINE
AN 2001374922 MEDLINE
DN 21324818 PubMed ID: 11430986
TI Structure--function characterization of cellulose synthase: relationship to other glycosyltransferases.
AU Saxena I M; Brown R M Jr; Dandekar T
CS Section of Molecular Genetics and Microbiology, School of Biological Sciences, University of Texas at Austin, Austin, TX 78712, USA.
SO PHYTOCHEMISTRY, (2001 Aug) 57 (7) 1135-48. Ref: 48
Journal code: 0151434. ISSN: 0031-9422.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200109
ED Entered STN: 20010924
Last Updated on STN: 20010924
Entered Medline: 20010920
AB A combined structural and functional model of the catalytic region of cellulose synthase is presented as a prototype for the action of processive beta-glycosyltransferases and other glycosyltransferases. A 285 amino acid segment of the Acetobacter xylinum cellulose synthase containing all the conserved residues in the globular region was subjected to **protein** modeling using the genetic algorithm. This region **folds** into a single large domain with a topology exhibiting a mixed alpha/beta **structure**. The **predicted** **structure** serves as a topological outline for the structure of this processive beta-glycosyltransferase. By incorporating new site-directed mutagenesis data and comparative analysis of the conserved aspartic acid residues and the QXXRW motif we deduce a number of functional implications based on the structure. This includes location of the UDP--glucose substrate-binding cavity, suggestions for the catalytic processing including positions of conserved and catalytic residues, secondary structure arrangement and domain organization. Comparisons to

cellulose synthases from higher plants (genetic algorithm based model for cotton CelA1), data from neural network predictions (PHD), and to the recently experimentally determined structures of the non-processive SpsA and beta 4-galactosyltransferase retest and further validate our structure-function description of this glycosyltransferase.

L4 ANSWER 6 OF 96 MEDLINE
AN 2001640253 MEDLINE
DN 21548623 PubMed ID: 11689334
TI Taking a functional genomics approach in molecular medicine.
AU Yaspo M L
CS Max Planck Institute for Molecular Genetics, Ihnestrasse 73, D-14195, Berlin, Germany.. yaspo@molgen.mpg.de
SO Trends Mol Med, (2001 Nov) 7 (11) 494-501. Ref: 70
Journal code: 100966035. ISSN: 1471-4914.
CY England: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200201
ED Entered STN: 20011107
Last Updated on STN: 20020129
Entered Medline: 20020128
AB The elucidation of genetic components of human diseases at the molecular level provides crucial information for developing future causal therapeutic intervention. High-throughput genome sequencing and systematic experimental approaches are fuelling strategic programs designed to investigate gene function at the biochemical, cellular and organism levels. Bioinformatics is one important tool in functional genomics, although showing clear limitations in **predicting** ab initio gene **structures**, gene function and **protein folds** from raw sequence data. Systematic large-scale data-set generation, using the same type of experiments that are used to decipher the function of single genes, are being applied on entire genomes. Comparative genomics, establishment of gene catalogues, and investigation of cellular and tissue molecular profiles are providing essential tools for understanding gene function in complex biological networks.

L4 ANSWER 7 OF 96 MEDLINE
AN 2001420985 MEDLINE
DN 21363291 PubMed ID: 11470603
TI Structural genomics: opportunities and challenges.
AU Mittl P R; Grutter M G
CS Institute of Biochemistry, University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland.
SO CURRENT OPINION IN CHEMICAL BIOLOGY, (2001 Aug) 5 (4) 402-8. Ref: 91
Journal code: 9811312. ISSN: 1367-5931.
CY England: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200109
ED Entered STN: 20010924
Last Updated on STN: 20010924
Entered Medline: 20010920
AB Following the complete genome sequencing of an increasing number of organisms, structural biology is engaging in a systematic approach of high-throughput structure determination called structural genomics to create a complete inventory of **protein folds/ structures** that will help **predict** functions for all **proteins**. First results show that structural genomics will be

highly effective in finding functional annotations for **proteins** of unknown function.

L4 ANSWER 8 OF 96 MEDLINE
AN 2001343630 MEDLINE
DN 21300006 PubMed ID: 11406409
TI LG/LNS domains: multiple functions -- one business end?.
AU Rudenko G; Hohenester E; Muller Y A
CS Howard Hughes Medical Institute and Dept of Biochemistry, University of Texas Southwestern Medical Center, Dallas, TX 75390-9050, USA.. rudenko@chop.swmed.edu
SO TRENDS IN BIOCHEMICAL SCIENCES, (2001 Jun) 26 (6) 363-8. Ref: 37
Journal code: 7610674. ISSN: 0968-0004.
CY England: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200108
ED Entered STN: 20010813
Last Updated on STN: 20010813
Entered Medline: 20010809
AB The three-dimensional structures of LG/LNS domains from neurexin, the laminin alpha 2 chain and sex hormone-binding globulin reveal a close structural relationship to the carbohydrate-binding pentraxins and other lectins. However, these LG/LNS domains appear to have a preferential ligand-interaction site distinct from the carbohydrate-binding sites found in lectins, and this interaction site accommodates not only sugars but also steroids and **proteins**. In fact, the LG/LNS domain interaction site has features reminiscent of the antigen-combining sites in immunoglobulins. The LG/LNS domain presents an interesting case in which the **fold** has remained conserved but the functional sites have evolved; consequently, making **predictions** of **structure**-function relationships on the basis of the lectin **fold** alone is difficult.

L4 ANSWER 9 OF 96 MEDLINE
AN 2001503121 MEDLINE
DN 21436030 PubMed ID: 11551181
TI **Fold** predictions for bacterial genomes.
AU Pawlowski K; Rychlewski L; Zhang B; Godzik A
CS AstraZeneca R&D Lund, Lund, S-221 87, Sweden.
SO JOURNAL OF STRUCTURAL BIOLOGY, (2001 May-Jun) 134 (2-3) 219-31. Ref: 80
Journal code: 9011206. ISSN: 1047-8477.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200110
ED Entered STN: 20010913
Last Updated on STN: 20011029
Entered Medline: 20011025
AB **Fold** assignments for newly sequenced genomes belong to the most important and interesting applications of the booming field of **protein structure prediction**. We present a brief survey and a discussion of such assignments completed to date, using as an example several **fold** assignment projects for **proteins** from the Escherichia coli genome. This review focuses on steps that are necessary to go beyond the simple assignment projects and into the development of tools extending our understanding of functions of **proteins** in newly sequenced genomes. This paper also discusses several problems seldom addressed in the literature, such as the problem

of domain prediction and complementary predictions (e.g., transmembrane regions and flexible regions) and cross-correlation of predictions from different servers. The influence of sequence and **structure** database growth on **prediction** success is also addressed. Finally, we discuss the perspectives of the field in the context of massive sequence and structure determination projects, as well as the development of novel prediction methods.

L4 ANSWER 10 OF 96 MEDLINE
AN 2001200057 MEDLINE
DN 21183950 PubMed ID: 11286964
TI Homologues of archaeal rhodopsins in plants, animals and fungi: structural and functional predications for a putative fungal chaperone **protein**.
AU Zhai Y; Heijne W H; Smith D W; Saier M H Jr
CS Department of Biology, University of California at San Diego, 9500 Gilman Drive, 92093-0116, La Jolla, CA, USA.
NC 5RO1 AI21702 (NIAID)
9RO1 GM55434 (NIGMS)
SO BIOCHIMICA ET BIOPHYSICA ACTA, (2001 Apr 2) 1511 (2) 206-23. Ref: 60
Journal code: 0217513. ISSN: 0006-3002.
CY Netherlands
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200105
ED Entered STN: 20010529
Last Updated on STN: 20010529
Entered Medline: 20010521
AB The microbial rhodopsins (MR) are homologous to putative chaperone and retinal-binding **proteins** of fungi. These **proteins** comprise a coherent family that we have termed the MR family. We have used modeling techniques to **predict** the **structure** of one of the putative yeast chaperone **proteins**, YRO2, based on homology with bacteriorhodopsins (BR). Availability of the structure allowed depiction of conserved residues that are likely to be of functional significance. The results lead us to predict an extracellular **protein folding** function and a transmembrane proton transport pathway. We suggest that **protein folding** is energized by a novel mechanism involving the proton motive force. We further show that MR family **proteins** are distantly related to a family of fungal, animal and plant **proteins** that include the human lysosomal cystine transporter (LCT) of man (cystinosin), mutations in which cause cystinosis. Sequence and phylogenetic analyses of both the MR family and the LCT family are reported. **Proteins** in both families are of the same approximate size, exhibit seven putative transmembrane alpha-helical spanners (TMSs) and show limited sequence similarity. We show that the LCT family arose by an internal gene duplication event and that TMSs 1-3 are homologous to TMSs 5-7. Although the same could not be demonstrated statistically for MR family members, homology with the LCT family suggests (but does not prove) a common evolutionary pathway. Thus, TMSs 1-3 and 5-7 in both LCT and MR family members may share a common origin, accounting for their shared structural features.

=> d 11-20 bib ab

L4 ANSWER 11 OF 96 MEDLINE
AN 2001503118 MEDLINE
DN 21436027 PubMed ID: 11551178
TI Functional inferences from blind ab initio **protein**

structure predictions.
AU Bonneau R; Tsai J; Ruczinski I; Baker D
CS Department of Biochemistry, University of Washington, Seattle, Washington 98195, USA.
SO JOURNAL OF STRUCTURAL BIOLOGY, (2001 May-Jun) 134 (2-3) 186-90. Ref: 34
Journal code: 9011206. ISSN: 1047-8477.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200110
ED Entered STN: 20010913
Last Updated on STN: 20011029
Entered Medline: 20011025
AB Ab initio **protein structure prediction** methods have improved dramatically in the past several years. Because these methods require only the sequence of the **protein** of interest, they are potentially applicable to the open reading frames in the many organisms whose sequences have been and will be determined. Ab initio methods cannot currently produce models of high enough resolution for use in rational drug design, but there is an exciting potential for using the methods for functional annotation of **protein** sequences on a genomic scale. Here we illustrate how functional insights can be obtained from low-resolution **predicted structures** using examples from blind ab initio **structure predictions** from the third and fourth critical assessment of **structure prediction** (CASP3, CASP4) experiments.

L4 ANSWER 12 OF 96 MEDLINE
AN 2001681227 MEDLINE
DN 21581301 PubMed ID: 11727705
TI [A turning point in the knowledge of the structure-function-activity relations of elastin].
Un tournant essentiel dans la connaissance des relations structure--fonction--activite de l'elastine.
AU Alix A J
CS Universite de Reims Champagne-Ardenne (URCA), Institut Federatif de Recherches FR53 Biomolecules, Faculte des Sciences Exactes et Naturelles, B.P. 1039, 51 687 Reims, Champagne, France.. alain.alix@univ-reims.fr
SO JOURNAL DE LA SOCIETE DE BIOLOGIE, (2001) 195 (2) 181-93. Ref: 34
Journal code: 100890617.
CY France
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA French
FS Priority Journals
EM 200201
ED Entered STN: 20011203
Last Updated on STN: 20020129
Entered Medline: 20020128
AB In this review are presented the last new results of our research group dealing with the molecular structures (atomic level) of tropoelastin, elastin and elastin derived peptides studied by using essentially methods of bioinformatics (theoretical predictions and molecular modelling) linked to experimental circular dichroism spectroscopic studies. We already had characterized both the local secondary structure and some parts of the tertiary structure of the tropoelastin and elastin molecules (human, bovine...), by using either theoretical **predictions** (local secondary **structure**, linear epitopes...) and/or experimental data (optical spectroscopic methods: Raman scattering, infrared absorption, circular dichroism). Except the cross-linking regions which

are in helical conformations, the whole tropoelastin structure displays a lot of beta-reverse turns which usually belong to irregular structures in **proteins**. These turns play a key role in other regularly structures orientation (alpha-helix, beta-strand), thus they are very important in the native **protein** 3D architecture. It is particularly true for human tropoelastin, because its sequence is rich in glycines and prolines, and these residues are frequently met in beta-turns (a beta-turn is made of four consecutive residues which are stabilized by an hydrogen bond). Several types of beta-turns can be defined with the dihedral angles values phi and psi of the two central residues. Thus, by using a very recent updated set of propensities for the amino acid residues to belong to given types of reverse beta-turns (extracted from a reference set of known 3-D structures of globular **proteins**), we have determined, (by using our home made software COUDES), for all possible tetrapeptides of the human tropoelastin sequence, the distribution and the characterization of the possible type of turns. Thus, it is shown that the locations and/or the types of these reverse beta-turns reveal a regularity and are not all random. This confirms our hypothesis that intra-molecular elasticity of tropoelastin could be explained by the possibility of transitions between conformations involving short beta-strands and beta-turns. This result is of great interest in the construction (by using molecular biology) of elastic biomaterials derived from the elastin sequence (particularly, the elastin derived peptides corresponding to the sequence exon 21--(exon 24--exon 24...). Our study permit also to predict the conformations of specific elastin derived peptides which could have interesting biological activity. Peptides resulting from the degradation of elastin, the insoluble polymer of tropoelastin and responsible for the elasticity of vertebrate tissues, can induce biological effects and notably the regulation of matrix metalloproteinases (MMP-s) activity. Recently, it was proposed that some elastin derived hexapeptides resulting from circular permutations of VGVAPG (a three **fold** repetition sequence in exon 24 of human tropoelastin) possess MMP-1 production and activation regulation properties. This effect depends on the presence of the tropoelastin specific membraneous receptor 67 KDa EBP (Elastin Binding **Protein**). Our results obtained by using both circular dichroism spectroscopy and linear predictions confirmed the hypothesis of a structure dependent mechanism with a possibly occurring type VIII beta-turn on the first four residues of the GXXPG sequence consensus which is only present among all active peptides. Thus, we have performed extensive molecular dynamics studies, in both implicit and explicit solvent, on these active and inactive elastin derived hexapeptides. Using our own analysis method of pattern recognition of the types of the beta-reverse-turns followed during the molecular dynamics trajectory, we found that active and inactive peptides effectively form two well distinct conformational groups in which active peptides preferentially adopt conformation close to type VIII GXXP (beta-reverse-turn. The structural role of the C terminal G residue could also be explained. Additional molecular simulations on (VGVAPG)2 and (VGVAPG)3 show the formation of two or three GXXP tetrapeptides adopting a structure close to type VIII beta-reverse-turn, suggesting a local conformational preference for this motif. This observation of a specific structural single and/or repeated motif is in agreement with the circular dichroism spectra of the involved (VGVAPG)1, (VGVAPG)2 and (VGVAPG)3 peptides and then it can be proposed that their biological activities have to be linear. The final aim of this type of work is to understand more about the sequence/structure/function/activity relationships of those structured peptides in order to propose specific sequences (corresponding to specific structures) for best biological activity results.

L4 ANSWER 13 OF 96 MEDLINE
AN 2001448542 MEDLINE
DN 21237929 PubMed ID: 11340057
TI Ab initio **protein structure prediction**: progress and prospects.
AU Bonneau R; Baker D

CS Department of Biochemistry, University of Washington, Seattle, Washington, Box 357350, 98195, USA.. dabaker@u.washington.edu
SO ANNUAL REVIEW OF BIOPHYSICS AND BIOMOLECULAR STRUCTURE, (2001) 30 173-89. Ref: 90
Journal code: 9211097. ISSN: 1056-8700.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200108
ED Entered STN: 20010813
Last Updated on STN: 20010813
Entered Medline: 20010809
AB Considerable recent progress has been made in the field of ab initio **protein structure prediction**, as witnessed by the third Critical Assessment of **Structure Prediction** (CASP3). In spite of this progress, much work remains, for the field has yet to produce consistently reliable ab initio **structure prediction** protocols. In this work, we review the features of current ab initio protocols in an attempt to highlight the foundations of recent progress in the field and suggest promising directions for future work.

L4 ANSWER 14 OF 96 MEDLINE
AN 2001245538 MEDLINE
DN 21109762 PubMed ID: 11179902
TI Integration of genome data and **protein structures**: **prediction** of **protein folds**, **protein** interactions and "molecular phenotypes" of single nucleotide polymorphisms.
AU Sunyaev S; Lathe W 3rd; Bork P
CS European Molecular Biology Laboratory (EMBL), Meyerhofstrasse 1, 69117 Heidelberg, Germany.. sunyaev@embl-heidelberg.de
SO CURRENT OPINION IN STRUCTURAL BIOLOGY, (2001 Feb) 11 (1) 125-30. Ref: 48
Journal code: 9107784. ISSN: 0959-440X.
CY England: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200105
ED Entered STN: 20010517
Last Updated on STN: 20010517
Entered Medline: 20010510
AB With the massive amount of sequence and structural data being produced, new avenues emerge for exploiting the information therein for applications in several fields. **Fold** distributions can be mapped onto entire genomes to learn about the nature of the **protein** universe and many of the interactions between **proteins** can now be predicted solely on the basis of the genomic context of their genes. Furthermore, by utilising the new incoming data on single nucleotide polymorphisms by mapping them onto three-dimensional structures of **proteins**, problems concerning population, medical and evolutionary genetics can be addressed.

L4 ANSWER 15 OF 96 MEDLINE
AN 2001640464 MEDLINE
DN 21548847 PubMed ID: 11690649
TI Predicting **protein** conformation by statistical methods.
AU Simon I; Fiser A; Tusnady G E
CS Institute of Enzymology, BRC, Hungarian Academy of Sciences, Budapest, Hungary.. simon@enzim.hu

SO BIOCHIMICA ET BIOPHYSICA ACTA, (2001 Oct 18) 1549 (2) 123-36. Ref: 119
Journal code: 0217513. ISSN: 0006-3002.
CY Netherlands
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200112
ED Entered STN: 20011107
Last Updated on STN: 20020123
Entered Medline: 20011207
AB The unique **folded** structure makes a **polypeptide** a functional **protein**. The number of known sequences is about a hundred times larger than the number of known structures and the gap is increasing rapidly. The primary goal of all **structure prediction** methods is to obtain structure-related information on **proteins**, whose structures have not been determined experimentally. Besides this goal, the development of accurate prediction methods helps to reveal principles of **protein folding**. Here we present a brief survey of **protein structure predictions** based on statistical analyses of known sequence and structure data. We discuss the background of these methods and attempt to elucidate principles, which govern structure formation of soluble and membrane **proteins**.

L4 ANSWER 16 OF 96 MEDLINE
AN 2001700314 MEDLINE
DN 21615649 PubMed ID: 11747907
TI The architecture of parallel beta-helices and related **folds**.
AU Jenkins J; Pickersgill R
CS Institute of Food Research, Norwich Research Park, Colney Lane, Norwich NR4 7UA, UK.. john.jenkins@bbsrc.ac.uk
SO PROGRESS IN BIOPHYSICS AND MOLECULAR BIOLOGY, (2001 Oct) 77 (2) 111-75. Ref: 198
Journal code: 0401233. ISSN: 0079-6107.
CY England: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, ACADEMIC)
LA English
FS Priority Journals
EM 200203
ED Entered STN: 20011219
Last Updated on STN: 20020305
Entered Medline: 20020304
AB Three-dimensional structures have been determined of a large number of **proteins** characterized by a repetitive **fold** where each of the repeats (coils) supplies a strand to one or more parallel beta-sheets. Some of these **proteins** form superfamilies of **proteins**, which have probably arisen by divergent evolution from a common ancestor. The classical example is the family including four families of pectinases without obviously related primary sequences, the phage P22 tailspike endorhamnosidase, chrondroitinase B and possibly pertactin from Bordetella pertusis. These show extensive stacking of similar residues to give aliphatic, aromatic and polar stacks such as the asparagine ladder. This suggests that coils can be added or removed by duplication or deletion of the DNA corresponding to one or more coils and explains how homologous **proteins** can have different numbers of coils.This process can also account for the evolution of other families of **proteins** such as the beta-rolls, the leucine-rich repeat **proteins**, the hexapeptide repeat family, two separate families of beta-helical antifreeze **proteins** and the spiral **folds**. These families need not be related to each other but will share features such as relative untwisted beta-sheets, stacking of similar residues and

turns between beta-strands of approximately 90 degrees often stabilized by hydrogen bonding along the direction of the parallel beta-helix.Repetitive **folds** present special problems in the comparison of structures but offer attractive targets for **structure prediction**. The stacking of similar residues on a flat parallel beta-sheet may account for the formation of amyloid with beta-strands at right-angles to the fibril axis from many unrelated peptides.

L4 ANSWER 17 OF 96 MEDLINE
AN 2001416529 MEDLINE
DN 21358283 PubMed ID: 11465730
TI **Protein structure prediction** in genomics.
CM Comment in: Brief Bioinform. 2001 May;2(2):108-10
AU Jones D T
CS Department of Biological Sciences, Brunel University, Uxbridge, UK.. David.Jones@brunel.ac.uk
SO Brief Bioinform, (2001 May) 2 (2) 111-25. Ref: 58
Journal code: 100912837. ISSN: 1467-5463.
CY England: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200109
ED Entered STN: 20010910
Last Updated on STN: 20010910
Entered Medline: 20010906
AB As the number of completely sequenced genomes rapidly increases, including now the complete Human Genome sequence, the post-genomic problems of genome-scale **protein** structure determination and the issue of gene function identification become ever more pressing. In fact, these problems can be seen as interrelated in that experimentally determining or **predicting** or the **structure** of **proteins** encoded by genes of interest is one possible means to glean subtle hints as to the functions of these genes. The applicability of this approach to gene characterisation is reviewed, along with a brief survey of the reliability of large-scale **protein structure prediction** methods and the prospects for the development of new prediction methods.

L4 ANSWER 18 OF 96 MEDLINE
AN 2001234067 MEDLINE
DN 21111909 PubMed ID: 11166648
TI **Protein structure prediction**.
AU Al-Lazikani B; Jung J; Xiang Z; Honig B
CS Department of Biochemistry and Molecular Biophysics, Howard Hughes Medical Institute, Columbia University, 630 West 168th Street, New York, NY 10032, USA.
NC GM30518 (NIGMS)
SO CURRENT OPINION IN CHEMICAL BIOLOGY, (2001 Feb) 5 (1) 51-6. Ref: 52
Journal code: 9811312. ISSN: 1367-5931.
CY England: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200105
ED Entered STN: 20010517
Last Updated on STN: 20010517
Entered Medline: 20010503
AB The **prediction** of **protein structure**, based primarily on sequence and structure homology, has become an increasingly important activity. Homology models have become more accurate and their

range of applicability has increased. Progress has come, in part, from the flood of sequence and structure information that has appeared over the past few years, and also from improvements in analysis tools. These include profile methods for sequence searches, the use of three-dimensional structure information in sequence alignment and new homology modeling tools, specifically in the prediction of loop and side-chain conformations. There have also been important advances in understanding the physical chemical basis of **protein** stability and the corresponding use of physical chemical potential functions to identify correctly **folded** from incorrectly **folded** **protein** conformations.

L4 ANSWER 19 OF 96 MEDLINE
AN 2000492215 MEDLINE
DN 20442068 PubMed ID: 10985762
TI Topology, stability, sequence, and length: defining the determinants of two-state **protein folding** kinetics.
AU Plaxco K W; Simons K T; Ruczinski I; Baker D
CS Department of Chemistry and Biochemistry and Interdepartmental Program in Biochemistry and Molecular Biology, University of California, Santa Barbara, Santa Barbara, California 93106, USA.. kwp@chem.ucsb.edu
SO BIOCHEMISTRY, (2000 Sep 19) 39 (37) 11177-83. Ref: 65
Journal code: 0370623. ISSN: 0006-2960.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200010
ED Entered STN: 20001027
Last Updated on STN: 20001027
Entered Medline: 20001019
AB The fastest simple, single domain **proteins fold** a million times more rapidly than the slowest. Ultimately this broad kinetic spectrum is determined by the amino acid sequences that define these **proteins**, suggesting that the mechanisms that underlie **folding** may be almost as complex as the sequences that encode them. Here, however, we summarize recent experimental results which suggest that (1) despite a vast diversity of structures and functions, there are fundamental similarities in the **folding** mechanisms of single domain **proteins** and (2) rather than being highly sensitive to the finest details of sequence, their **folding** kinetics are determined primarily by the large-scale, redundant features of sequence that determine a **protein**'s gross structural properties. That **folding** kinetics can be **predicted** using simple, empirical, **structure**-based rules suggests that the fundamental physics underlying **folding** may be quite straightforward and that a general and quantitative theory of **protein folding** rates and mechanisms (as opposed to unfolding rates and thus **protein** stability) may be near on the horizon.

L4 ANSWER 20 OF 96 MEDLINE
AN 2000400249 MEDLINE
DN 20295850 PubMed ID: 10836143
TI Nicotinic receptors at the amino acid level.
AU Corringer P J; Le Novere N; Changeux J P
CS Unite de recherche associee au Centre National de la Recherche Scientifique D1284 Institut Pasteur, Paris, France.
SO ANNUAL REVIEW OF PHARMACOLOGY AND TOXICOLOGY, (2000) 40 431-58. Ref: 167
Journal code: 7607088. ISSN: 0362-1642.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)

(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200008
ED Entered STN: 20000824
Last Updated on STN: 20000824
Entered Medline: 20000817
AB nAChRs are pentameric transmembrane **proteins** into the superfamily of ligand-gated ion channels that includes the 5HT3, glycine, GABAA, and GABAC receptors. Electron microscopy, affinity labeling, and mutagenesis experiments, together with secondary **structure predictions** and measurements, suggest an all-beta **folding** of the N-terminal extracellular domain, with the connecting loops contributing to the ACh binding pocket and to the subunit interfaces that mediate the allosteric transitions between conformational states. The ion channel consists of two distinct elements symmetrically organized along the fivefold axis of the molecule: a barrel of five M2 helices, and on the cytoplasmic side five loops contributing to the selectivity filter. The allosteric transitions of the **protein** underlying the physiological ACh-evoked activation and desensitization possibly involve rigid body motion of the extracellular domain of each subunit, linked to a global reorganization of the transmembrane domain responsible for channel gating.

=> d 21-30 bib ab

L4 ANSWER 21 OF 96 MEDLINE
AN 2001077570 MEDLINE
DN 20421823 PubMed ID: 10968613
TI Perspectives in inorganic structural biology: solution structures of metalloproteins.
AU Banci L; Presenti C
CS CERM and Department of Chemistry, University of Florence, Sesto Fiorentino, Italy.. banci@cerm.unifi.it
SO JOURNAL OF BIOLOGICAL INORGANIC CHEMISTRY, (2000 Aug) 5 (4) 422-31. Ref: 158
Journal code: 9616326. ISSN: 0949-8257.
CY GERMANY: Germany, Federal Republic of
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200101
ED Entered STN: 20010322
Last Updated on STN: 20010322
Entered Medline: 20010111
AB The achievements in the structural characterization in solution, through NMR spectroscopy, of **proteins** containing metal ions are reviewed and discussed. We call this branch "inorganic structural biology". The results of this approach are presented here for cytochrome b5, used in this paper as a case system. These results are discussed particularly in the light of their relevance for understanding the biological function of the **proteins**. Furthermore, the extension of the characterization to the internal motions and to the **folding**/unfolding processes, as well as the development of tools for **structure prediction**, are critically presented. The message is that the complete characterization of a biological molecule cannot be limited to a static description of the structure but it should go beyond, analyzing the internal motions occurring at various time scales as well as the behavior in different conditions, such as in the presence of denaturing agents.

L4 ANSWER 22 OF 96 MEDLINE
AN 2001041026 MEDLINE

DN 20400938 PubMed ID: 10940251
TI Comparative **protein** structure modeling of genes and genomes.
AU Marti-Renom M A; Stuart A C; Fiser A; Sanchez R; Melo F; Sali A
CS Laboratories of Molecular Biophysics, Pels Family Center for Biochemistry and Structural Biology, Rockefeller University, New York, NY 10021, USA.
NC GM 54762 (NIGMS)
SO ANNUAL REVIEW OF BIOPHYSICS AND BIOMOLECULAR STRUCTURE, (2000) 29 291-325. Ref: 213
Journal code: 9211097. ISSN: 1056-8700.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, ACADEMIC)
LA English
FS Priority Journals
EM 200012
ED Entered STN: 20010322
Last Updated on STN: 20010322
Entered Medline: 20001207
AB Comparative modeling **predicts** the three-dimensional **structure** of a given **protein** sequence (target) based primarily on its alignment to one or more **proteins** of known **structure** (templates). The **prediction** process consists of **fold** assignment, target-template alignment, model building, and model evaluation. The number of **protein** sequences that can be modeled and the accuracy of the predictions are increasing steadily because of the growth in the number of known **protein** structures and because of the improvements in the modeling software. Further advances are necessary in recognizing weak sequence-structure similarities, aligning sequences with structures, modeling of rigid body shifts, distortions, loops and side chains, as well as detecting errors in a model. Despite these problems, it is currently possible to model with useful accuracy significant parts of approximately one third of all known **protein** sequences. The use of individual comparative models in biology is already rewarding and increasingly widespread. A major new challenge for comparative modeling is the integration of it with the torrents of data from genome sequencing projects as well as from functional and structural genomics. In particular, there is a need to develop an automated, rapid, robust, sensitive, and accurate comparative modeling pipeline applicable to whole genomes. Such large-scale modeling is likely to encourage new kinds of applications for the many resulting models, based on their large number and completeness at the level of the family, organism, or functional network.

L4 ANSWER 23 OF 96 MEDLINE
AN 2000165299 MEDLINE
DN 20165299 PubMed ID: 10700142
TI Structural genomics and its importance for gene function analysis.
AU Skolnick J; Fetrow J S; Kolinski A
CS Laboratory of Computational Genomics, The Danforth Plant Science Center, 893 N, Warson Rd., St. Louis, MO 63141, USA.. skolnick@danforthcenter.org
SO NATURE BIOTECHNOLOGY, (2000 Mar) 18 (3) 283-7. Ref: 59
Journal code: 9604648. ISSN: 1087-0156.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200005
ED Entered STN: 20000518
Last Updated on STN: 20000518
Entered Medline: 20000510
AB Structural genomics projects aim to solve the experimental structures of all possible **protein folds**. Such projects entail a

conceptual shift from traditional structural biology in which structural information is obtained on known **proteins** to one in which the structure of a **protein** is determined first and the function assigned only later. Whereas the goal of converting **protein** structure into function can be accomplished by traditional sequence motif-based approaches, recent studies have shown that assignment of a **protein**'s biochemical function can also be achieved by scanning its structure for a match to the geometry and chemical identity of a known active site. Importantly, this approach can use low-resolution structures provided by contemporary **structure prediction** methods. When applied to genomes, structural information (either experimental or predicted) is likely to play an important role in high-throughput function assignment.

L4 ANSWER 24 OF 96 MEDLINE
AN 2000219680 MEDLINE
DN 20219680 PubMed ID: 10753815
TI Ab initio **protein folding**.
AU Osguthorpe D J
CS Department of Chemistry, University of Bath, Bath, BA2 7AY, UK..
djosg@mgu.bath.ac.uk
SO CURRENT OPINION IN STRUCTURAL BIOLOGY, (2000 Apr) 10 (2) 146-52. Ref: 63
Journal code: 9107784. ISSN: 0959-440X.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200006
ED Entered STN: 20000622
Last Updated on STN: 20000622
Entered Medline: 20000612
AB Ab initio **protein folding** methods have been developing rapidly over the past few years and, at the last Critical assessment of methods of **protein structure prediction** (CASP) meeting, it was shown that important progress has been made in generating structure from sequence. Both methods based on statistical potentials and methods using physics-based potentials have shown improvements. Most current methods use statistics-based potentials and the development of these is ongoing. Additionally, the inclusion of multiple sequence data in the algorithms in order to aid in finding the native structure is a common theme. The use of physics-based potentials is less developed, which means that less progress has been made in understanding why a sequence forms a structure.

L4 ANSWER 25 OF 96 MEDLINE
AN 2000219679 MEDLINE
DN 20219679 PubMed ID: 10753811
TI Effective energy functions for **protein structure prediction**.
AU Lazaridis T; Karplus M
CS Department of Chemistry, City College of CUNY, New York, NY 10031, USA..
themis@sci.ccny.edu
SO CURRENT OPINION IN STRUCTURAL BIOLOGY, (2000 Apr) 10 (2) 139-45. Ref: 78
Journal code: 9107784. ISSN: 0959-440X.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200006
ED Entered STN: 20000622
Last Updated on STN: 20000622

Entered Medline: 20000612

AB **Protein structure prediction, fold** recognition, homology modeling and design rely mainly on statistical effective energy functions. Although the theoretical foundation of such functions is not clear, their usefulness has been demonstrated in many applications. Molecular mechanics force fields, particularly when augmented by implicit solvation models, provide physical effective energy functions that are beginning to play a role in this area.

L4 ANSWER 26 OF 96 MEDLINE
AN 2000145556 MEDLINE
DN 20145556 PubMed ID: 10679345
TI Structural energetics of **protein folding** and binding.
AU Edgcomb S P; Murphy K P
CS Department of Biochemistry, University of lowa, lowa City, IA 52246, USA.
SO CURRENT OPINION IN BIOTECHNOLOGY, (2000 Feb) 11 (1) 62-6. Ref: 44
Journal code: 9100492. ISSN: 0958-1669.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200003
ED Entered STN: 20000327
Last Updated on STN: 20000327
Entered Medline: 20000310
AB Structural energetics is a method for calculating the energetics of **protein folding** and binding reactions as a function of temperature. This approach allows measured energetics to be interpreted with regards to the **protein structure** and the **prediction** of energetics from known structures. Recent advances include improvements in the parameterization of enthalpy, entropy and heat capacity terms and new applications, especially with regards to understanding dynamic properties of **proteins** and how these are affected by ligand binding.

L4 ANSWER 27 OF 96 MEDLINE
AN 2000134914 MEDLINE
DN 20134914 PubMed ID: 10670018
TI Structural biology.
AU Holmes K C
CS Max-Planck-Institut fur medizinische Forschung, Heidelberg, Germany..
holmes@mpimf-heidelberg.mpg.de
SO PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY OF LONDON. SERIES B: BIOLOGICAL SCIENCES, (1999 Dec 29) 354 (1352) 1977-84. Ref: 32
Journal code: 7503623. ISSN: 0962-8436.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200003
ED Entered STN: 20000407
Last Updated on STN: 20000407
Entered Medline: 20000330
AB **Protein** crystallography has become a major technique for understanding cellular processes. This has come about through great advances in the technology of data collection and interpretation, particularly the use of synchrotron radiation. The ability to express eukaryotic genes in Escherichia coli is also important. Analysis of known structures shows that all **proteins** are built from about 1000 primeval **folds**. The collection of all primeval **folds** provides a basis for **predicting structure** from

sequence. At present about 450 are known. Of the presently sequenced genomes only a fraction can be related to known **proteins** on the basis of sequence alone. Attempts are being made to determine all (or as many as possible) of the structures from some bacterial genomes in the expectation that structure will point to function more reliably than does sequence. Membrane **proteins** present a special problem. The next 20 years may see the experimental determination of another 40,000 **protein** structures. This will make considerable demands on synchrotron sources and will require many more biochemists than are currently available. The availability of massive structure databases will alter the way biochemistry is done.

L4 ANSWER 28 OF 96 MEDLINE
AN 1999395259 MEDLINE
DN 99395259 PubMed ID: 10464088
TI Global optimization of clusters, crystals, and biomolecules.
AU Wales D J; Scheraga H A
CS University Chemical Laboratories, Lensfield Road, Cambridge, CB2 1EW, UK.. dw34@cus.cam.ac.uk
SO SCIENCE, (1999 Aug 27) 285 (5432) 1368-72. Ref: 63
Journal code: 0404511. ISSN: 0036-8075.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 199909
ED Entered STN: 19990925
Last Updated on STN: 20000303
Entered Medline: 19990914
AB Finding the optimal solution to a complex optimization problem is of great importance in many fields, ranging from **protein structure prediction** to the design of microprocessor circuitry. Some recent progress in finding the global minima of potential energy functions is described, focusing on applications of the simple "basin-hopping" approach to atomic and molecular clusters and more complicated hypersurface deformation techniques for crystals and biomolecules. These methods have produced promising results and should enable larger and more complex systems to be treated in the future.

L4 ANSWER 29 OF 96 MEDLINE
AN 2000070834 MEDLINE
DN 20070834 PubMed ID: 10600698
TI **Predicting protein** three-dimensional **structure**
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AU Moult J
CS Center for Advanced Research in Biotechnology, University of Maryland Biotechnology Institute, Rockville, MD 20850, USA.. moult@umbi.umd.edu
SO CURRENT OPINION IN BIOTECHNOLOGY, (1999 Dec) 10 (6) 583-8. Ref: 53
Journal code: 9100492. ISSN: 0958-1669.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 200001
ED Entered STN: 20000114
Last Updated on STN: 20000114
Entered Medline: 20000105
AB The current state of the art in modeling **protein** structure has been assessed, based on the results of the CASP (Critical Assessment of **protein Structure Prediction**) experiments. In comparative modeling, improvements have been made in sequence alignment,

sidechain orientation and loop building. Refinement of the models remains a serious challenge. Improved sequence profile methods have had a large impact in **fold** recognition. Although there has been some progress in alignment quality, this factor still limits model usefulness. In ab initio **structure prediction**, there has been notable progress in building approximately correct structures of 40-60 residue-long **protein** fragments. There is still a long way to go before the general ab initio prediction problem is solved. Overall, the field is maturing into a practical technology, able to deliver useful models for a large number of sequences.

L4 ANSWER 30 OF 96 MEDLINE
AN 1999290837 MEDLINE
DN 99290837 PubMed ID: 10361096
TI Progress in **protein structure prediction**: assessment of CASP3.
AU Sternberg M J; Bates P A; Kelley L A; MacCallum R M
CS Biomolecular Modelling Laboratory, Imperial Cancer Research Fund, London, UK.. m.sternberg@icrf.icnet.uk
SO CURRENT OPINION IN STRUCTURAL BIOLOGY, (1999 Jun) 9 (3) 368-73. Ref: 34
Journal code: 9107784. ISSN: 0959-440X.
CY ENGLAND: United Kingdom
DT Conference; Conference Article; (CONGRESSES)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 199907
ED Entered STN: 19990727
Last Updated on STN: 20000303
Entered Medline: 19990712
AB The third comparative assessment of techniques of **protein structure prediction** (CASP3) was held during 1998. This is a blind trial in which **structures** are **predicted** prior to having knowledge of the coordinates, which are then revealed to enable the assessment. Three sections at the meeting evaluated different methodologies - comparative modelling, **fold** recognition and ab initio methods. For some, but not all of the target coordinates, high quality models were submitted in each of these sections. There have been improvements in prediction techniques since CASP2 in 1996, most notably for ab initio methods.

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L4 ANSWER 31 OF 96 MEDLINE
AN 2000020733 MEDLINE
DN 20020733 PubMed ID: 10550212
TI Intrinsically unstructured **proteins**: re-assessing the **protein** structure-function paradigm.
AU Wright P E; Dyson H J
CS Department of Molecular Biology and Skaggs Institute of Chemical Biology, The Scripps Research Institute, 10550 North Torrey Pines Road, La Jolla, CA 92037, USA.. wright@scrips.edu
NC DK34909 (NIDDK)
GM36643 (NIGMS)
GM57374 (NIGMS)
SO JOURNAL OF MOLECULAR BIOLOGY, (1999 Oct 22) 293 (2) 321-31. Ref: 93
Journal code: 2985088R. ISSN: 0022-2836.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals

EM 199911
ED Entered STN: 20000111
Last Updated on STN: 20000111
Entered Medline: 19991119
AB A major challenge in the post-genome era will be determination of the functions of the encoded **protein** sequences. Since it is generally assumed that the function of a **protein** is closely linked to its three-dimensional **structure**, **prediction** or experimental determination of the library of **protein** structures is a matter of high priority. However, a large proportion of gene sequences appear to code not for **folded**, globular **proteins**, but for long stretches of amino acids that are likely to be either unfolded in solution or adopt non-globular structures of unknown conformation. Characterization of the conformational propensities and function of the non-globular **protein** sequences represents a major challenge. The high proportion of these sequences in the genomes of all organisms studied to date argues for important, as yet unknown functions, since there could be no other reason for their persistence throughout evolution. Clearly the assumption that a **folded** three-dimensional structure is necessary for function needs to be re-examined. Although the functions of many **proteins** are directly related to their three-dimensional structures, numerous **proteins** that lack intrinsic globular structure under physiological conditions have now been recognized. Such **proteins** are frequently involved in some of the most important regulatory functions in the cell, and the lack of intrinsic structure in many cases is relieved when the **protein** binds to its target molecule. The intrinsic lack of structure can confer functional advantages on a **protein**, including the ability to bind to several different targets. It also allows precise control over the thermodynamics of the binding process and provides a simple mechanism for inducibility by phosphorylation or through interaction with other components of the cellular machinery. Numerous examples of domains that are unstructured in solution but which become structured upon binding to the target have been noted in the areas of cell cycle control and both transcriptional and translational regulation, and unstructured domains are present in **proteins** that are targeted for rapid destruction. Since such **proteins** participate in critical cellular control mechanisms, it appears likely that their rapid turnover, aided by their unstructured nature in the unbound state, provides a level of control that allows rapid and accurate responses of the cell to changing environmental conditions.

L4 ANSWER 32 OF 96 MEDLINE
AN 1999338994 MEDLINE
DN 99338994 PubMed ID: 10410805
TI Membrane **protein folding** and stability: physical principles.
AU White S H; Wimley W C
CS Department of Physiology and Biophysics, University of California at Irvine 92697-4560, USA.. blanco@helium.biomol.uci.edu
NC GM46823 (NIGMS)
SO ANNUAL REVIEW OF BIOPHYSICS AND BIOMOLECULAR STRUCTURE, (1999) 28 319-65.
Ref: 188
Journal code: 9211097. ISSN: 1056-8700.
CY United States
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, ACADEMIC)
LA English
FS Priority Journals
EM 199909
ED Entered STN: 19990921
Last Updated on STN: 19990921
Entered Medline: 19990908

AB Stably **folded** membrane **proteins** reside in a free energy minimum determined by the interactions of the peptide chains with each other, the lipid bilayer hydrocarbon core, the bilayer interface, and with water. The **prediction** of three-dimensional **structure** from sequence requires a detailed understanding of these interactions. Progress toward this objective is summarized in this review by means of a thermodynamic framework for describing membrane **protein folding** and stability. The framework includes a coherent thermodynamic formalism for determining and describing the energetics of peptide-bilayer interactions and a review of the properties of the environment of membrane **proteins**--the bilayer milieu. Using a four-step thermodynamic cycle as a guide, advances in three main aspects of membrane **protein folding** energetics are discussed: **protein** binding and **folding** in bilayer interfaces, transmembrane helix insertion, and helix-helix interactions. The concepts of membrane **protein** stability that emerge provide insights to fundamental issues of **protein folding**.

L4 ANSWER 33 OF 96 MEDLINE
AN 2000020730 MEDLINE
DN 20020730 PubMed ID: 10550209
TI **Protein folding**: from the levinthal paradox to **structure prediction**.
AU Honig B
CS Department of Biochemistry and Molecular Biophysics, Columbia University, 630 West 168 St., New York, NY 10032, USA.. bh6@columbia.edu
NC GM 30518 (NIGMS)
SO JOURNAL OF MOLECULAR BIOLOGY, (1999 Oct 22) 293 (2) 283-93. Ref: 73
Journal code: 2985088R. ISSN: 0022-2836.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 199911
ED Entered STN: 20000111
Last Updated on STN: 20000111
Entered Medline: 19991119
AB This article is a personal perspective on the developments in the field of **protein folding** over approximately the last 40 years. In addition to its historical aspects, the article presents a view of the principles of **protein folding** with particular emphasis on the relationship of these principles to the problem of **protein structure prediction**. It is argued that despite much that is new, the essential elements of our current understanding of **protein folding** were anticipated by researchers many years ago. These elements include the recognition of the central importance of the **polypeptide** backbone as a determinant of **protein** conformation, hierarchical **protein folding**, and multiple **folding** pathways. Important areas of progress include a detailed characterization of the **folding** pathways of a number of **proteins** and a fundamental understanding of the physical chemical forces that determine **protein** stability. Despite these developments, **fold** prediction algorithms still encounter difficulties in identifying the correct **fold** for a given sequence. This may be due to the possibility that the free energy differences between at least a few alternate conformations of many **proteins** are not large. Significant progress in **protein structure prediction** has been due primarily to the explosive growth of sequence and structural databases. However, further progress is likely to depend in part on the ability to combine information available from databases with principles and algorithms derived from physical chemical studies of **protein folding**. An approach to the integration of the two areas is

outlined with specific reference to the PrISM program that is a fully integrated sequence/structural-analysis/**fold**-recognition/homology model building software system.

L4 ANSWER 34 OF 96 MEDLINE
AN 2000020729 MEDLINE
DN 20020729 PubMed ID: 10550208
TI How RNA **folds**.
AU Tinoco I Jr; Bustamante C
CS Department of Chemistry, University of California Berkeley, Berkeley, CA 94720-1460, USA.
NC GM 10840 (NIGMS)
GM 32543 (NIGMS)
SO JOURNAL OF MOLECULAR BIOLOGY, (1999 Oct 22) 293 (2) 271-81. Ref: 55
Journal code: 2985088R. ISSN: 0022-2836.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 199911
ED Entered STN: 20000111
Last Updated on STN: 20000111
Entered Medline: 19991119
AB We describe the RNA **folding** problem and contrast it with the much more difficult **protein folding** problem. RNA has four similar monomer units, whereas **proteins** have 20 very different residues. The **folding** of RNA is hierarchical in that secondary structure is much more stable than tertiary **folding**. In RNA the two levels of **folding** (secondary and tertiary) can be experimentally separated by the presence or absence of Mg2+. Secondary **structure** can be **predicted** successfully from experimental thermodynamic data on secondary structure elements: helices, loops, and bulges. Tertiary interactions can then be added without much distortion of the secondary structure. These observations suggest a **folding** algorithm to **predict** the **structure** of an RNA from its sequence. However, to solve the RNA **folding** problem one needs thermodynamic data on tertiary structure interactions, and identification and characterization of metal-ion binding sites. These data, together with force versus extension measurements on single RNA molecules, should provide the information necessary to test and refine the proposed algorithm.

L4 ANSWER 35 OF 96 MEDLINE
AN 1999257335 MEDLINE
DN 99257335 PubMed ID: 10322219
TI **Predicting structures** for genome **proteins**.
AU Fischer D; Eisenberg D
CS Faculty of Natural Science, Department of Math and Computer Science, Beer-Sheva, 84015, Israel.. dfischer@cs.bgu.ac.il
SO CURRENT OPINION IN STRUCTURAL BIOLOGY, (1999 Apr) 9 (2) 208-11. Ref: 22
Journal code: 9107784. ISSN: 0959-440X.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 199908
ED Entered STN: 19990910
Last Updated on STN: 20000303
Entered Medline: 19990820

AB Assigning three-dimensional **protein folds** to genome sequences is essential to understanding **protein** function. Although experimental three-dimensional structures are currently available for only a very small fraction of these sequences, computational **fold** assignment is able to assign **folds** to 20-30% of the sequences in various genomes. This percentage varies depending on the particular organism under analysis, on the sensitivities of the methods used and on the number of experimental structures available at the time the assignment is carried out. The fraction of assignable sequences is currently increasing at an annual rate of roughly 18%. If this rate is sustained throughout the coming years, three-dimensional computational models for more than half of the genome sequences may be available by the year 2003.

L4 ANSWER 36 OF 96 MEDLINE
AN 2000048330 MEDLINE
DN 20048330 PubMed ID: 10581629
TI [**Predicting** the secondary **structures** of the ribonucleic acids (RNA)].
Przewidywanie struktur drugorzedowych kwasow rybonukleinowych (RNA).
AU Ziomek K; Kierzek R
CS Instytut Chemii Bioorganicznej PAN, Poznan.
SO POSTEPY BIOCHEMII, (1999) 45 (2) 74-80. Ref: 19
Journal code: 0023525. ISSN: 0032-5422.
CY Poland
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA Polish
FS Priority Journals
EM 200001
ED Entered STN: 20000124
Last Updated on STN: 20000124
Entered Medline: 20000111

L4 ANSWER 37 OF 96 MEDLINE
AN 1999375593 MEDLINE
DN 99375593 PubMed ID: 10446500
TI Genome-based structural biology.
AU Frishman D; Mewes H W
CS GSF-Forschungszentrum fuer Umwelt und Gesundheit, Munich Information Center for Protein Sequences, am Max-Planck-Institut fur Biochemie, Martinsried, Germany.. frishman@mips.biochem.mpg.de
SO PROGRESS IN BIOPHYSICS AND MOLECULAR BIOLOGY, (1999) 72 (1) 1-17. Ref: 78
Journal code: 0401233. ISSN: 0079-6107.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 199908
ED Entered STN: 19990910
Last Updated on STN: 19990910
Entered Medline: 19990826
AB Spectacular achievements in whole genome sequencing open up new possibilities for structural research. **Protein** structures can now be studied in their natural genomic context. On the other hand, **structure prediction** algorithms can be improved using species-specific tendencies in **folding** patterns. Finally, efficient strategies to select targets for structure determination can be devised. In this review we consider new computational approaches and results in **protein** structure analysis stemming from the availability of complete genomes.

L4 ANSWER 38 OF 96 MEDLINE
AN 1999089220 MEDLINE
DN 99089220 PubMed ID: 9872054
TI Contemporary approaches to **protein** structure classification.
AU Swindells M B; Orengo C A; Jones D T; Hutchinson E G; Thornton J M
CS Helix Research Institute, Kisarazu, Japan.
SO BIOESSAYS, (1998 Nov) 20 (11) 884-91. Ref: 53
Journal code: 8510851. ISSN: 0265-9247.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals; Space Life Sciences
EM 199901
ED Entered STN: 19990202
Last Updated on STN: 20000303
Entered Medline: 19990121
AB In a similar manner to sequence database searching, it is also possible to compare three-dimensional **protein** structure. Such methods can be extremely useful because a structural similarity may represent a distant evolutionary relationship that is undetectable by sequence analysis. In this review, we summarise the most popular structure comparison methods, show how they can be used for database searching, and then describe some of the most advanced attempts to develop comprehensive **protein** structure classifications. With such data, it is possible to identify distant evolutionary relationships, provide libraries of unique **folds** for **structure prediction**, estimate the total number of **folds** that exist, and investigate the preference for certain types of structures over others.

L4 ANSWER 39 OF 96 MEDLINE
AN 1998330762 MEDLINE
DN 98330762 PubMed ID: 9666333
TI **Protein fold** irregularities that hinder sequence analysis.
AU Russell R B; Ponting C P
CS SmithKline Beecham Pharmaceuticals, Bioinformatics, New Frontiers Science Park (North), Essex, UK.. russelr1@mh.uk.sbphrd.com
SO CURRENT OPINION IN STRUCTURAL BIOLOGY, (1998 Jun) 8 (3) 364-71. Ref: 70
Journal code: 9107784. ISSN: 0959-440X.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals; Space Life Sciences
EM 199809
ED Entered STN: 19981008
Last Updated on STN: 19981008
Entered Medline: 19980925
AB The detection of homologous **protein** sequences frequently provides useful **predictions** of function and **structure**. Methods for homology searching have continued to improve, such that very distant evolutionary relationships can now be detected. Little attention has been paid, however, to the problems of detecting homology when domains are inserted or permuted. Here we review recent occurrences of these phenomena and discuss methods that permit their detection.

L4 ANSWER 40 OF 96 MEDLINE
AN 1998228369 MEDLINE
DN 98228369 PubMed ID: 9560336
TI **Protein folding**: think globally, (inter)act locally.
CM Comment in: Curr Biol. 1998 Jul 2;8(14):R478-9
AU Gross M

CS Oxford Centre for Molecular Sciences, New Chemistry Laboratory, Oxford,OX1 3QT, UK.
SO CURRENT BIOLOGY, (1998 Apr 23) 8 (9) R308-9. Ref: 12
Journal code: 9107782. ISSN: 0960-9822.
CY ENGLAND: United Kingdom
DT Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)
LA English
FS Priority Journals
EM 199808
ED Entered STN: 19980828
Last Updated on STN: 20000303
Entered Medline: 19980818
AB **Protein folding** appears to be almost too complex for a complete description or for accurate **structure prediction** from sequence data. A simple way of analysing local interactions, however, bears promise of linking theory with experiment and cutting through some of the complexities.

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FULL ESTIMATED COST	23.04	23.25

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